Extension of the MolMod Database to Transferable Force Fields

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Abstract

MolMod, a web-based database for classical force fields for molecular simulations of fluids [Mol. Sim. 45, 10 (2019) 806-814], was extended to transferable force fields. Eight transferable force fields, including all-atom and united-atom type force fields, were implemented in the MolMod database: OPLS-UA, OPLS-AA, COMPASS, CHARMM, GROMOS, TraPPE, Potoff, and TAMie. These transferable force fields cover a large variety of chemical substance classes. The system is designed such that new transferable force fields can be readily integrated. A graphical user interface was implemented that enables constructing molecules. The MolMod database compiles the force field for the specified component and force field type and provides the corresponding data and meta data as well as ready-to-use input files for the molecule for different simulation engines. This helps the user to flexibly choose molecular models and integrate them swiftly in their individual workflows – reducing risks of input errors in molecular simulations.

Introduction

Molecular simulations with force fields have become an important tool for predicting thermophysical properties[1–10] as well as for studying nanoscopic processes[11–18] in many scientific disciplines. The link of the simulations to the real world is established by the employed substance models, i.e. by the force fields. They provide mathematical expressions describing the interactions between the particles on the molecular level and are usually formulated as interaction potentials between different interaction sites. Therein, the interaction sites describe atoms or groups of atoms. The choice of the force field is decisive for the reliability of the predictions obtained from the molecular simulation.[19–22] A large number of force fields has been proposed in the past decades. Yet, their electronic accessibility and findability[23,24] is still cumbersome. Despite the abundant importance of force fields for molecular simulations, data science principles such as FAIR[23] (findable, accessible, interoperable, and reusable) have received limited attention by the molecular simulation community. Therefore, there is a lack of data standards and electronically available models. This also affects the reproducibility of molecular simulation computer experiments, which has been identified as a problem in recent years.[25–30] The lack of force field databases for finding and reusing force field models has been stressed in the past.[24]

Two types of force fields can be distinguished: (i) component-specific force fields and (ii) transferable force fields. Component-specific force fields are substance models that were individually designed and parameterized for modeling a given substance. Hence, component-specific force fields describe solely the molecular interactions of a particular chemical substance. The generalization of a component-specific force field to chemically related or similar substances is in general not feasible.

Transferable force fields[31–34] on the other hand are generalized chemical construction plans that can be used for building a large number of substance models based on transferable building blocks. Hence, the interaction parameters of the sites of a transferable force field can be applied to a variety of chemical substances. Usually, the parametrization of the building block parameters is carried out with a limited number of components and the obtained force field parameters are then transferred to other substances containing the same building blocks. Therefore, the development of transferable force fields is a demanding and tedious task. Transferable force fields can be considered as a construction plan for building component-specific force fields. Thus, transferable force fields are powerful tools that are today widely used in the molecular simulation community.

Among transferable force fields, there are different approaches to model the atomistic architecture. Three types of force fields are often distinguished: all-atom (AA), united-atom (UA), and coarse-grained (CG) force fields.[35] In AA force fields, all atoms are represented by individual interaction sites. In contrast, UA force fields combine multiple atoms to one interaction site. Mostly, $\mathrm{CH_x}$ groups are modeled as one interaction site in which the H atoms are only implicitly modeled. In CG force fields, larger molecule segments (or multiple molecules) are merged into a single interaction site.

The strength of transferable force fields lies in their generalized description of molecular sub-structures using building blocks. However, the flexibility and wide applicability generally comes at the cost of a loss of accuracy in the description compared to component-specific models. Moreover, transferable force fields comprise a high level of abstraction and challenges in the usability.[27] To the best of our knowledge, no broad data base for transferable force fields of fluids has been established yet. Some force field databases are available,[36–39] but they mostly cover just one specific transferable force field (usually developed by the creators of the respective database) or potential models for solid states.[40]

Therefore, in this work, a broad database for transferable force fields was developed and implemented in the existing MolMod database,[41] which so far only considered component-specific force fields. Fig. 1 gives an overview of the structure of the MolMod Database including the ’component specific’ part as well as the ’transferable’ part presented in this work. The two parts share the same front end, but have individual back end kernels and data structures.

The *MolMod Transferable* database is able to handle both AA and UA force fields. Table 1 gives an overview of the transferable force fields that are presently implemented in the MolMod database. Presently, *MolMod Transferable* contains eight transferable force fields, namely: TraPPE,[31] TAMie,[42] Potoff,[43] COMPASS,[44] CHARMM,[45] GROMOS,[46] OPLS-AA,[32] and OPLS-UA.[47] These force fields were taken from the literature and cover in general different chemical substance classes (details are given below). The data infrastructure of *MolMod Transferable* uses the force field data ontology and data format proposed in Refs.[48–50] Based on these interoperable data standards, further transferable force fields can readily be integrated into the MolMod database. A graphical user interface is provided on the website that can be used for defining a molecular structure. The websites directly displays the transferable force field parameters for that given molecule based on a chosen transferable force field. Moreover, *MolMod Transferable* provides input files for different simulation engines that can be downloaded in different formats.

This paper is organized as follows: First, the operating principles of *MolMod Transferable* are explained. Then, the implementation of the force fields and the available input formats are described. Afterwards, comments on the data infrastructure, data management, and data integrity are given. Finally, the work is summarized and an outlook to future work is presented.

MolMod Transferable

The *MolMod Transferable* database can be accessed at `https://molmod.boltzmann-zuse.de/`. The purpose of *MolMod Transferable* is to provide findable, accessible, and interoperable access to force field models for molecules based on transferable force fields. The main task of *MolMod Transferable* is to build a component-specific force field for a given molecule based on a given transferable force field and provide simulation engine input files. The workflow of *MolMod Transferable* is depicted in Fig. 2. The *user input* (left side of Fig. 2) consists of the specification of the molecule and the transferable force field to be used. The molecule specification is to be provided by specifying the molecule structure, i.e. the geometry of the atoms. The geometry of the molecule can be specified by a drawing of the structural formula or by providing a MOL file.[51] The drawing can be done by the ChemDoodle sketcher,[52] which is integrated into the *MolMod* website. Additionally, the user has to select a transferable force field among those currently available in the *MolMod* database.

MolMod displays the component-specific force field model for the considered molecule on-the-fly on the front end of the website. For identifying the functional groups of a given molecule, an algorithm based on the method proposed by *Ertl*[53] was implemented in *MolMod Transferable*. The kernel of *MolMod Transferable* builds a component-specific force field model by assigning the model parameters from the generalized transferable construction plans to a concrete molecular structure. Presently, *MolMod Transferable* covers only molecules that can be represented by the scheme of *Kanagalingam et al.*,[50] which comprises a large number organic substances. As all force fields considered here (see below for details) are based on groups that are covered in the scheme of *Kanagalingam et al.*[50] If this is the case, the component-specific force field can be built; elsewise the user is informed by the website that the transferable force field cannot be used in the present case. Changes of the molecular structure via the structure drawing tool or changing the transferable force field are quasi-instantaneously depicted on the website. Both, the data of the force field and the meta-data are displayed on the website. The actual force field data consists of the force field parameters, i.e. variables and their numeric values and units that define the interaction sites, the initial configuration, and the intermolecular as well as the intramolecular potentials acting between the interaction sites. The meta-data of a user-built component-specific force field comprises the information on the references that published the transferable force field parameters in use for the given model. For some molecules, this might be multiple publications, e.g. for an alcohol where the methyl and methylene group parameters were published separately from the hydroxyl group parameters. Moreover, input files for MD or MC simulation engines of the component-specific force field model built by the user are directly provided by the *MolMod* database.

Besides being a tool for simulators, the *MolMod Transferable* database is also a useful tool for force field developers to distribute newly developed force fields. The force field parameters in the *MolMod Transferable* database are stored in the generalized data format proposed in Ref.[50] The format is both human readable and interoperable with *MolMod Transferable*. Thus, it is straightforward to integrate new transferable force fields into the *MolMod Transferable* database. Details on the implementation of force fields and the general workflow too upload new force fields are given in Sec. and .

Fig. 3 shows a screenshot of the user interface of the *MolMod Transferable* front end. The *MolMod Transferable* front end consists of five sections (top to bottom). In the user input section (highlighted in red in Fig. 3), which is entitled *Builder*, the user specifies the structure of the molecule by drawing the structure formula or providing a MOL file as well as specifies the transferable force field via a drop-down menu.

The section *Overview* (highlighted in green in Fig. 3) contains meta-data information on the component-specific force field including the molecular formula, identifiers for the references used for building the model, the number of interaction sites in the force field, and the name of the underlying transferable force field.

The *Force Field* section (highlighted in blue in Fig. 3) contains the full specification of the actual component-specific force field by providing its parameters in separate tables. The first sub-section contains the specification of the sites and the equilibrium configuration, the second and third sub-sections contain the specifications of the inter- and intramolecular interactions.

In the first sub-section, the first table *Sites* provides a list of the interaction sites, their names, their functional groups as well as their molar masses. In the second table, the *Initial Configuration* is given (xyz-coordinates of each interaction site in an equilibrium configuration). Details on the calculation of the initial configuration are given in Sec. . The

Intermolecular Potential Parameters sub-section provides the parameters for the intermolecular interactions. Depending on the types of interactions used in a given component-specific force field, corresponding tables are depicted, i.e. a table for the dispersive-repulsive interactions (e.g. Lennard-Jones or Mie potential parameters) and a table for charges and multipoles (no charges are applicable in the ethane model exemplaricly shown in Fig. 3). Also, a link to the nomenclature section of the *MolMod* database is given that provides details on the underlying mathematical equations used for the modeling of the interactions. The *Intramolecular Potential Parameters* sub-section provides the parameters for the intramolecular interactions as well as the specifications of intramolecular constraints. In this section, tables for the specification of the *Bond*, *Angle*, *Dihedral*, and *Improper* interactions are displayed (latter three are not applicable in the example shown in Fig. 3).

The individual tables contain all information needed to identify the interaction potential (an ID for each interaction type, the IDs and names of the sites that are part of the interaction, the potential ID, the actual potential parameters, the type of interaction (rigid or flexible), and the reference to the publication in which the parameters were first published).

In the *Downloads* section (highlighted in yellow in Fig. 3), *MolMod Transferable* provides files for download that contain the data and meta-data of the considered component-specific force field. Different file formats are available that correspond to input file formats of popular simulation engines. More details on the input files are given below in 'Data Management and Data Integrity'.

The last section *References* (highlighted in light blue in Fig. 3) provides the details on the literature sources that were used to construct the component-specific model. In some cases, it might contain only a single reference, but multiple references will be listed when the information was spread in several papers or if erratums were considered. The references are specified using the full author list, title, journal title, volume, page number, year, and the DOI number including a web-link.

Implemented Transferable Force Fields

MolMod Transferable covers both UA and AA transferable force fields. Table 1 gives an overview of the force fields presently implemented in *MolMod Transferable.* These transferable force fields differ significantly in the chemical groups for which parameters are available, cf. Table 2. Furthermore, the force fields were developed at different times, e.g. the OPLS-UA force field was in most parts developed in the 1980ies, whereas the Potoff and TAMie force field were developed in the past two decades. Transferable force fields presently implemented in *MolMod* database use the Lennard-Jones potential or the generalized Mie potential for modeling the dispersive-repulsive interactions and point charges for modeling the polarities for describing intermolecular interactions. For the intramolecular interactions, different approaches are used, i.e. some transferable force fields use constraint stretching and bending bonds (i.e. rigid), whereas other transferable force fields use harmonic springs for modeling the stretching and bending. Most force fields use a torsion potential for modeling the intramolecular rotations. Yet, different force fields mostly use different torsional potential functions.

The force fields are stored in the *MolMod* database using the data format proposed in our previous work.[50] This data format is based on tags that are attributed to every site and that contain information on the functional groups, the modeled atoms or group of atoms, the neighboring interaction sites, the number of bonds, and the highest bond order of the site. In particular, the data format provides a high interoperability and is well-defined,[50] which enables an easy integration of new force fields in the database. Presently, eight transferable force fields are integrated in *MolMod Transferable.* In the following a brief overview of these transferable force fields (cf. Table 1 and Table 2) is given. For some transferable force fields, multiple versions are available in the literature, i.e. multiple parameter sets for a given functional group have been proposed. In the *MolMod* database, only a single version for each transferable force field is implemented – as indicated by the references in Table 1.

The united-atom OPLS-UA transferable force field (Optimized Potentials for Liquid Simulations)[47] was developed by *Jorgensen and co-workers.* The basis of the OPLS-UA force field was published in 1984 and has been extended in the following years. Today, it can be applied to a wide range of structural groups (cf. Table 1). The intermolecular interactions are represented by charges and Lennard-Jones interaction sites. The bond lengths and bond angles are fixed in OPLS-UA. The bond length and bond bending angle values were determined using spectroscopic data. The intramolecular torsion is considered by explicit potentials and the potential parameters were obtained using quantum chemical data. Parameters for the charges and the non-bonded dispersive-repulsive interactions were optimized with respect to macroscopic thermodynamic data and structural data.

Also the all-atom OPLS-AA transferable force field[32] is implemented in the *MolMod* data base. It was also developed by *Jorgensen and co-workers* and is today widely used, e.g. in computational biology. For the OPLS-AA force field,[32] the bond and bending angle parameters were adopted from the AMBER[54] and the CHARMM force field.[55] The torsional potential parameters were fitted to QM data. The non-bonded dispersive-repulsive interaction parameters (modeled by the Lennard-Jones potential) and charges were fitted to thermodynamic and structural property data (in parts adopted from the OPLS-UA[47]).

The TraPPE-UA transferable force field (Transferable Potentials for Phase Equilibria) comprises a large number of functional group building blocks, cf. Table 1. It was developed by the *J.I. Siepmann* and co-workers.[36] In the *MolMod* database, presently the united-atom force field (TraPPE-UA) is implemented, ,which has to be distinguished from the all-atom force field TraPPE-AA.[56–58] The TraPPE-UA force field is today one of the most widely used transferable force fields, cf. Table 1. The basis of the TraPPE-UA force field was published in 1998 and has been substantially extended since. The non-bonded dispersive-repulsive interactions are represented by the classical Lennard-Jones potential. The Lennard-Jones interaction parameters were fitted to experimental data for the vapor-liquid equilibrium of selected components. The parameters for the charges and the intramolecular interactions were either taken from the literature or fitted to quantum-mechanical calculation results. In most cases, the bending parameters were adopted from AMBER;[54] the dihedral parameters as well as charge parameters were adopted from OPLS-UA.[47,59]

The COMPASS transferable force field (Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies) is an all-atom force field that was first published in 1998.[44] The force field was developed to describe simultaneously thermodynamic condensed phase properties and vibrational molecular properties. Hence, an important focus was also on the intramolecular interaction parameters.[35] Therefore, besides the bond, bending, dihedral, and improper interactions, also cross terms are included in the transferable force field. These cross terms model the coupling between the different intramolecular interactions, e.g. the bond-bond, bond-angle, angle-angle, bond-torsion, and angle-torsion couplings. The bond and angle potentials are described by functions with quartic terms. The dispersive-repulsive interactions are modeled by a 9-6 Mie potential. The parameters of the COMPASS force field were determined from a fit to QM data (charges and intramolecular potentials) and to thermodynamic liquid state properties (dispersive-repulsive potential).

The all-atom CHARMM transferable force field (Chemistry at HARvard Macromolecular Mechanics) version C22/CMAP[45] is implemented in the *MolMod* database. The CHARMM force field was originally developed for modeling bio-molecules such as lipids and proteins, but is today also used for other applications. The CHARMM force field is one of the most popular force fields, cf. Table 1. As for most force fields, the intramolecular parameters were fitted to structural data. Therefore, data from different spectroscopic methods were used in addition to ab-initio QM data. The charges were fitted to QM data. The dispersive-repulsive interaction parameters were fitted to experimental solvation data for model compounds in water. As a water model, TIP3P[60] was used in the optimization process.

The united-atom GROMOS transferable force field (Groningen Molecular Simulation) was developed by *W.F. Van Gunsteren* and *H.J. Berendsen* and co-workers and was primarily designed for describing aqueous bio-molecular systems. In the *MolMod* database, the GROMOS version 45A3[61] is implemented. The intermolecular parameters of the 45A3

GROMOS version were fitted to experimental data for the bulk liquid density, the enthalpy of vaporization, and the free energy of hydration. The simple point charge (SPC)[62] water model was used in the optimization process. The intramolecular parameters of the 45A3 GROMOS version were adopted from earlier versions, where they were in most parts fitted to quantum chemical data and in parts fine-tuned to macroscopic liquid phase properties.[61]

The Potoff transferable force field,[43] named here after the principal developer, *J. Potoff*, was first published in 2009. Compared to other transferable force fields, the Potoff force field presently comprises only a small number of functional group building blocks, such that alkanes, alkenes, and alkynes as well as perfluoralkanes, perfluoralkenes, and perfluoralkynes can be modeled. The Potoff force field uses the Mie potential for modeling the dispersive-repulsive interactions. The Mie parameters were fitted to experimental vapor-liquid equilibrium data. The intramolecular potential parameters were adopted from the TraPPE force field. The Potoff force field has recently been found to be remarkably accurate for predicting properties and state regions that were not considered in the model parametrization.[22]

The TAMie transferable force field (Transferable Anisotropic United-Atom Mie)[42] was developed by *J. Gross* and co-workers and uses the Mie potential for modeling the dispersive-repulsive interactions. For the TAMie force field, the intramolecular potential parameters were adopted from the TraPPE force field. In contrast to the TraPPE force field, the TAMie force field framework uses an anisotropic approach regarding the bond length between terminal methyl groups and neighboring interaction sites to better account for the hydrogen atoms. In its fitting procedure, parameters for the dispersive-repulsive interactions, partial charges, and the repulsive exponent of the Mie potential were simultaneously fitted to experimental vapor-liquid equilibrium data. The dispersive exponent was set to 6 in all cases.

Available input formats

The component-specific force fields built by *MolMod Transferable* can be directly downloaded by the user as input files for different common simulation engines. These input files contain the actual force field data written in the corresponding simulation engine syntax as well as the force field meta-data to make the input files transparently reusable.

Presently, *MolMod Transferable* provides download input files for three simulation engines, namely for LAMMPS,[63] *ms*2,[64,65] and Gromacs.[66] The files contain the calculated initial configuration of all sites as well as the force field parameters in the respective format for the molecule of interest.

The LAMMPS input files provided by the *MolMod* database consists of two files: The .int file contains the force field parameters for all types of interactions applicable to the model. It is written as a LAMMPS script file and, thus, can be readily integrated into any LAMMPS simulation script. The second file (`.molecule`) contains the geometry of the molecule (bond topology as well as the initial coordinates). For *ms*2, a `.pm` file is provided containing the geometry as well as the potential parameters. The Gromacs input files provided by *MolMod Transferable* consist of four `.itp` files containing the force field parameters, which are split into a main file, a file defining general force field properties, and two files for defining bonded and non-bonded interactions. Additionally, the initial coordinates are stored in a `.ptb` file.

Data Management and Data Integrity

In the following, the operating principle of the *MolMod* database for using transferable force fields and the corresponding data management system is presented. Fig. 4 shows schematically the interplay between the different database parts, users, and developers. The *MolMod* database is designed such that users can easily find and access force field data. For adding new force field models to the *MolMod* database, force field developers are invited to submit their force fields along with the corresponding meta-data to the *MolMod* developers (info.molmod@boltzmann-zuse.de). The data is then checked for consistency and integrated into the database. For submitting new force fields, the data format specified in Ref.[50] should be used, which is directly compatible with the *MolMod* database.

The *MolMod* database is hosted at the RPTU computer center. The *MolMod* database consists of two parts: The *MolMod* database website (highlighted in red in Fig. 4) and the actual database comprising the data and meta-data of the force fields (highlighted in blue in Fig. 4). The latter is stored in an SQL database. Both parts are stored in an individual Git repository, which provides a basic and robust data integrity level. The SQL database is setup within a Git repository that is updated once a day. Hence, a backup is written every 24 h and changes, that eventually crash the website or alter force field data, can be traced back. Also the code for the actual *MolMod* website is developed within a (separate) Git repository. Thereby, the integrated database system (cf. Fig. 4) is well maintainable and the data quality traceable. Moreover, the system is designed in a modular way such that it can be well extended, e.g. new transferable force fields can be easily integrated using the SQL data format defined in Ref.[50] and new user features implemented in the back end or front end of the website, e.g. new interaction potential functions.

The *MolMod* website itself consists of a back end and a front end (cf. Fig. 5). The back end contains the routines for building a component-specific force field based on the molecule structure specifications of the user and a transferable force field. Therefore, the back end retrieves the required force field parameters from the SQL database. Then, the back end builds the component-specific force field as well as determines an equilibrium configuration based on a heuristic approach that determines a (local) minimum of the total intramolecular potential energy.[67] Also, the back end constructs the simulation engine input files and carries out conversions, e.g. between xyz and internal coordinates and different multipole representations.[68] The results are then returned and depicted for the user on the front end.

Both the force field data and meta-data of *MolMod Transferable* are stored in an SQL database. The SQL database (here the version *MySQL 8.0.32* was used) contains the force field parameters within multiple tables (cf. Ref.[50] for details of the data architecture) for the sites, masses, bonds, angles, dihedrals, and special interactions, which also include references to the original publications using DOI identifiers. The data format[50] used in the SQL database generalizes the transferable force field construction plans such that different transferable force fields can be stored in a homogenized and well-defined machine readable way.

An overview of the internal operating principle for a user request for building a component-specific model for a given molecule structure are depicted in Fig. 5. Accordingly, the front end and the back end interact upon a user request. The molecule structure is in an intermediate step stored in an internal format that includes the information of the chemical groups and the molecule bonding structure. The molecular structure is converted into a collection of sites specifying chemical groups and their bonding structure. Based on this basic layout, the applicable types of intermolecular interactions and intramolecular interactions are identified. Then, a tag ID (following the data scheme embedded in the data format[50]) is assigned to each site according to the atom or group of atoms they represent, which also includes the information on the functional group they are part of. The details of this step evidently differ for united-atom and all-atom force fields. Based on the tags, the force field parameters for the intramolecular as well as intermolecular interactions are requested from the SQL database. That request is carried out for all implemented transferable force fields returning the information, which transferable force field actually contains parameters for all functional groups present in the molecule specified by the user. The information, which transferable force field is applicable for the considered component is then provided to the user via the force field drop down menu, cf. Fig. 3 – red colored section. Thereby, users can quickly screen the availability of force field models for a given substance.

Finally, the initial configuration of the considered molecule are computed based on the intramolecular force field potentials. Due to the increasing computational effort with increasing number of sites, the use of the *MolMod* database is only recommended for molecules up to

100 sites. Moreover, users have a limited open-access budget. Once all relevant parameters and the corresponding meta-data for a given component-specific force field are assigned and compiled, the data is sent to the front end and provided to the user. Moreover, the user can optionally request input files for different software packages. Such are created upon explicit user request to save computer time when input files are not required.

Exemplary Application

The application of the *MolMod Transferable* webpage is demonstrated in the following. Therefore, molecular dynamics simulations of n-decane ($C_{10}H_{22}$) at a temperature of $T = 373.15$ K and three pressures $p \in \{20, 90, 160\}$ MPa were conducted for each of the eight force fields. The force field were used as implemented in the *MolMod Transferable* database. For the TraPPE-UA, COMPASS, Potoff, and TAMie force field, simulations were carried out using LAMMPS. For the OPLS-UA, OPLS-AA, CHARMM, and GROMOS force field, simulations were carried out with Gromacs. All simulations were conducted in the NpT ensemble with 500 molecules. The time step was $\Delta\tau = 0.1$ fs. The simulations were equilibrated for 10^5 time steps. The production ran for 10^6 time steps. In the simulation with LAMMPS, the Nose-Hoover thermostat and barostat[69–71] were applied. In the Gromacs simulations, the Nose-Hoover thermostat[69,70] and the Parinello-Rahman barostat[72] were used.

Fig. 6 shows the results for the sampled density as function of the pressure in comparison with experimental data (experimental data points and correlation of experimental data). All considered force fields yield reasonable results for the density. It is out of the scope of this work to compare the performance of different force fields. Such comparisons have been carried out in the literature, e.g. Refs.[10,22]

Conclusions

In this work, the *MolMod* database was extended to transferable force fields. Therefore, a new workflow was developed and implemented that establishes a link between a user request for a component-specific force field for a given molecule and a transferable force field. The user specifies a molecule structure and a transferable force field; based on that, the database constructs the corresponding component-specific force field and provides both a comprehensive description as well as input files for popular molecular simulation engines. Various transferable force fields were included in *MolMod Transferable*, namely OPLS-UA, OPLS-AA, COMPASS, CHARMM, GROMOS, TraPPE, Potoff, and TAMie. The data architecture used to obtain a unified description of these models is based on a force field data standard developed in a recent work of our group.[50] Thereby, new transferable force fields can readily be integrated into the *MolMod* database. Force field developers are invited to submit their transferable force fields to the *MolMod* developers for integration in the database. *MolMod Transferable* provides ready-to-use input files for different popular molecular dynamics and Monte Carlo simulation engines. *MolMod Transferable* is open-access for the scientific community. Presently, *MolMod Transferable* comprises united-atom and all-atom force field frameworks. It would be interesting to extend this to coarse grain force fields in the future.

The development and maintenance of molecular simulation infrastructure such as the *MolMod* database is a highly interdisciplinary task. Experience in multiple programming languages, interfaces, data science aspects, chemistry, and computational physics are closely interconnected. *MolMod Transferable* provides a new level of accessibility and interoperability of transferable force fields, and, by reducing the risk of input errors, also to the reliability of molecular simulations based on transferable force fields.

Supporting Information Available

Comparison with literature data (PDF); Molecular Structure database (ZIP).

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Conflicts of Interest

There are no conflicts of interest to declare.

Data Availability

All molecular structure data used in the database is given in the electronic Supporting Information in a machine readable spread sheet format.

Author contribution statement

Sebastian Schmitt: Data Curation, Formal Analysis, Visualization, Methodology (equal), Writing/Review & Editing (equal); Gajanan Kanagalingam: Software (equal), Methodology (equal); Florian Fleckenstein: Data Curation, Formal Analysis (equal), Software (equal), Visualization (equal), Writing/Review & Editing (support); Daniel Froescher: Technical Support, Software (equal); Hans Hasse: Funding Acquisition (equal), Writing/Review &

Editing (support); Simon Stephan: Conceptualization, Methodology (lead), Supervision, Software (support), Writing/Original Draft Preparation (lead), Funding Acquisition (equal).

Figures & Tables

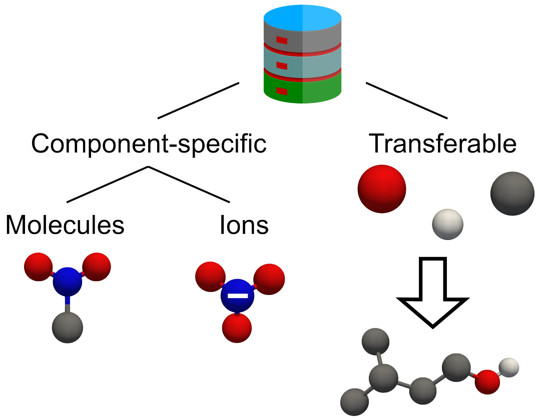


Figure 1: *MolMod* database consisting of the 'component-specific' part (left) and the new 'transferable' part.

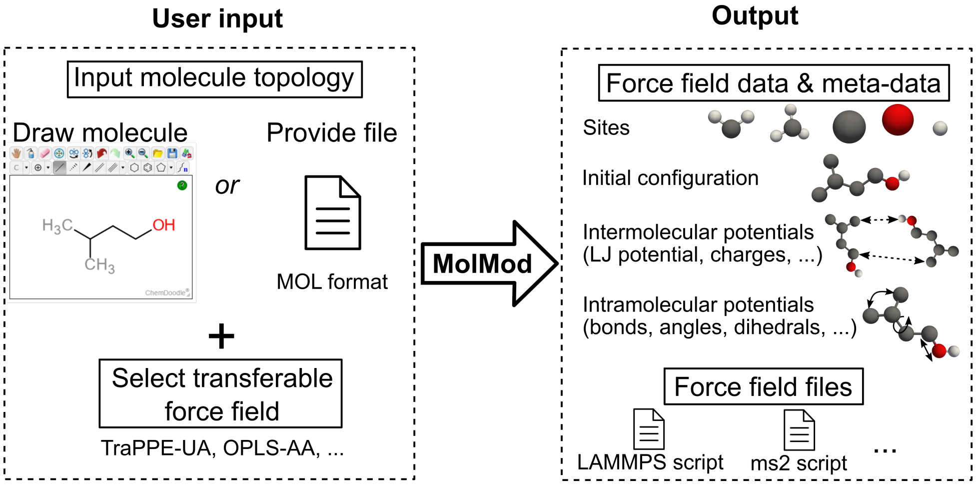
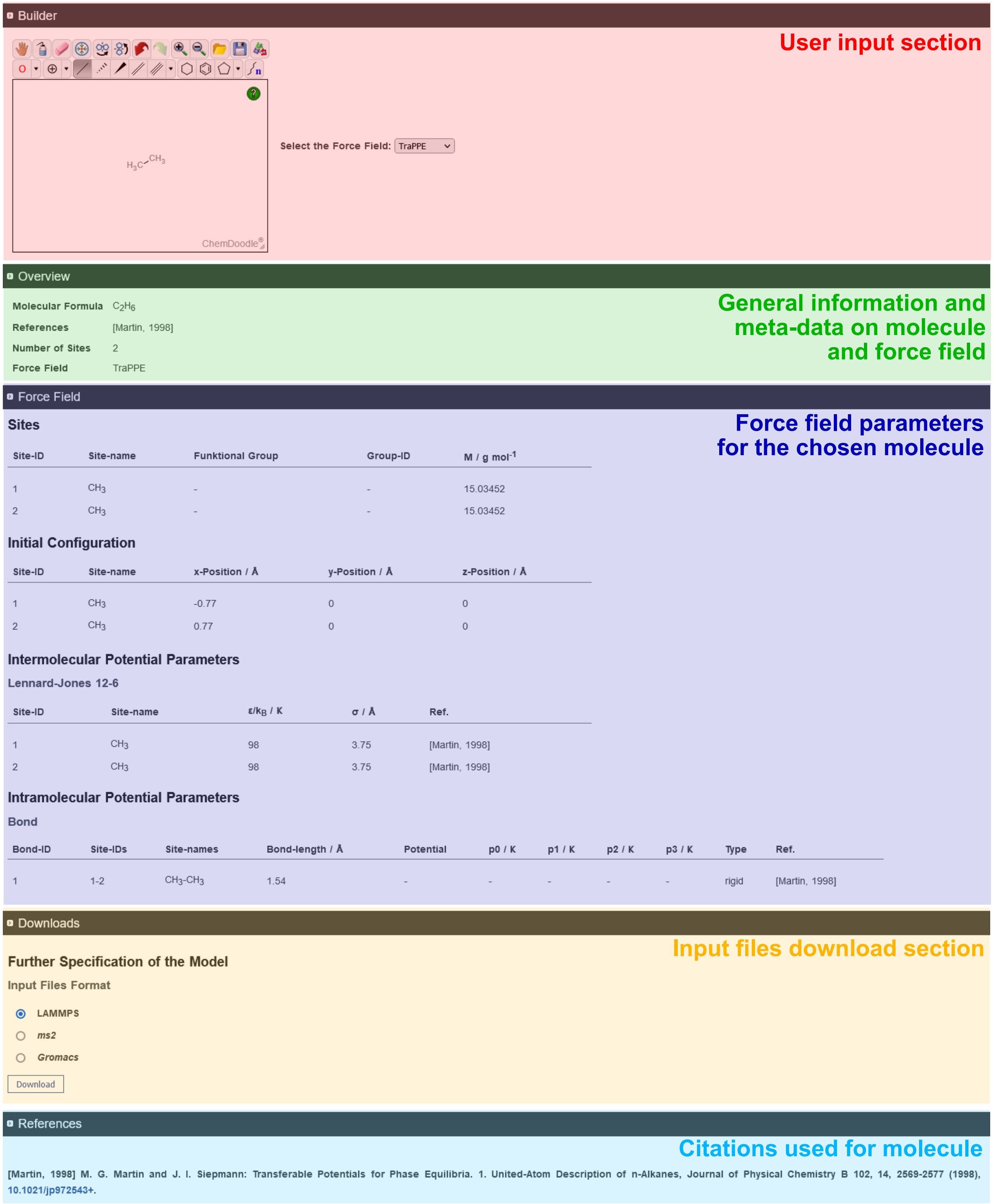


Figure 2: Workflow for users of *MolMod Transferable*.



Builder

User input section

Select the Force Field: TraPPE

Overview

General information and meta-data on molecule and force field

Molecular Formula	C_2H_6
References	[Martin, 1998]
Number of Sites	2
Force Field	TraPPE

Force Field

Force field parameters for the chosen molecule

Sites

Site-ID	Site-name	Funktional Group	Group-ID	M / g mol^{-1}
1	CH_3	-	-	15.03452
2	CH_3	-	-	15.03452

Initial Configuration

Site-ID	Site-name	x-Position / Å	y-Position / Å	z-Position / Å
1	CH_3	-0.77	0	0
2	CH_3	0.77	0	0

Intermolecular Potential Parameters

Lennard-Jones 12-6

Site-ID	Site-name	ε/k_B / K	σ / Å	Ref.
1	CH_3	98	3.75	[Martin, 1998]
2	CH_3	98	3.75	[Martin, 1998]

Intramolecular Potential Parameters

Bond

Bond-ID	Site-IDs	Site-names	Bond-length / Å	Potential	p0 / K	p1 / K	p2 / K	p3 / K	Type	Ref.
1	1-2	CH_3-CH_3	1.54	-	-	-	-	-	rigid	[Martin, 1998]

Downloads

Input files download section

Further Specification of the Model

Input Files Format

● LAMMPS

○ *ms2*

○ *Gromacs*

Download

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Citations used for molecule

[Martin, 1998] M. G. Martin and J. I. Siepmann: Transferable Potentials for Phase Equilibria. 1. United-Atom Description of n-Alkanes, Journal of Physical Chemistry B 102, 14, 2569-2577 (1998), 10.1021/jp972543+.

Figure 3: Screenshot of the user interface of the *MolMod Transferable* front end. As an example, the modeling of ethane C_2H_6 with the TraPPE-UA transferable force field is considered.

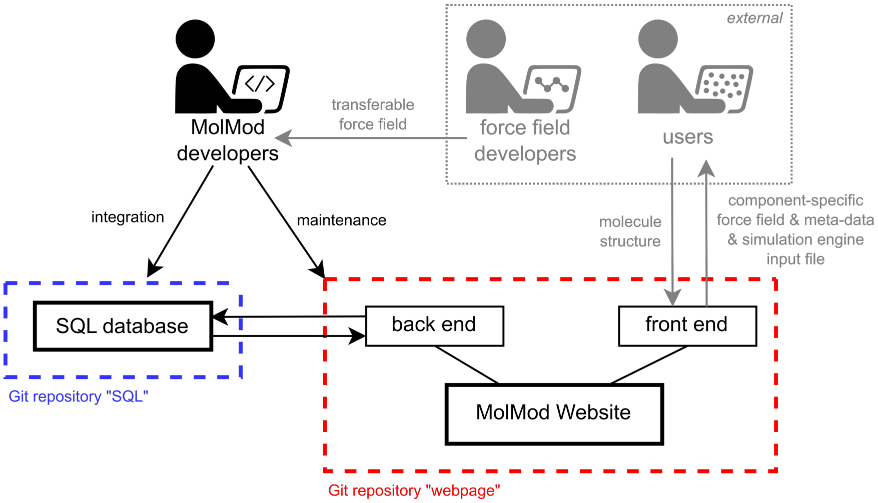

Figure 4: Operating principle of the *MolMod Transferable* database and the interaction of the admin, the user, and force field developers with the *MolMod Transferable* database.

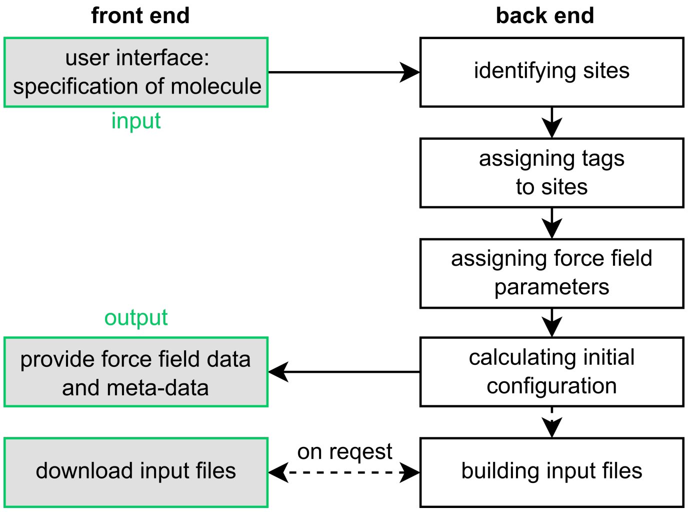

Figure 5: Operating principle of *MolMod Transferable* for a user request for building a component-specific force field for a given component based on a given transferable force field and providing an input file for a certain simulation engine.

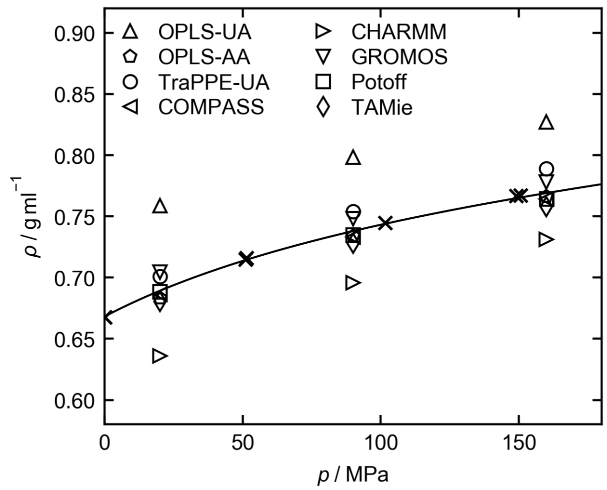

Figure 6: Density of n-decane as function of the pressure at T = 373 K. Open symbols: simulation results from eight different force fields; line: correlation to experimental data;[22] crosses: experimental values from Ref.[73]

Table 1: Overview of transferable force fields presently implemented in the *MolMod* database. Both, united-atom (UA) and all-atom (AA) force fields are available. Sorted chronologically. The number of citations was taken from the *Web of Science* (`https://www.webofscience.com`) as of June 26th, 2023. The number of citations is the sum of citations of the references given in the third column.

Name	**Type**	**References**	**First publication**	**Citations**
OPLS-UA	UA	[47,59,74–84]	1984	6433
OPLS-AA	AA	[32,85,86]	1996	11429
TraPPE-UA	UA	[31,87–97]	1998	5181
COMPASS	AA	[44]	1998	4406
CHARMM	AA	[45]	1998	11617
GROMOS	UA	[46]	2001	753
Potoff	UA	[43,98–100]	2009	150
TAMie	UA	[42,101–105]	2015	105

Table 2: Substance classes and functional groups implemented in the *MolMod* database (1st and 2nd column). The 3rd column lists the transferable force fields that comprise a given functional group.

Substance class	**Functional group**	**Force fields**
alkanes	CH_x–$\mathrm{CH}_x{}^{a}$	OPLS-UA, OPLS-AA, TraPPE-UA, COMPASS, CHARMM, GROMOS, Potoff, TAMie
alkenes	CH_x=$\mathrm{CH}_x{}^{b}$	OPLS-UA, TraPPE-UA, Potoff, TAMie
alkynes	$\mathrm{CH}_x \equiv \mathrm{CH}_x{}^{c}$	Potoff
(meth)acrylates	CH_x–O–C(=O)–CX=$\mathrm{CH}_2{}^{a,d}$	TraPPE-UA
alcohols	CH_x–O–H^{a}	OPLS-UA, OPLS-AA, TraPPE-UA, TAMie
aldehydes	X–C(–H)=$\mathrm{O}^{a,d}$	TraPPE-UA, TAMie
aromatic rings	CH–CH (arom.)	OPLS-AA, TraPPE-UA, CHARMM
cycloalkanes	CH_2–CH_2 (cyc.)	TraPPE-UA, GROMOS, TAMie
disulfides	CH_x–S–S–$\mathrm{CH}_x{}^{a}$	OPLS-UA, OPLS-AA, TraPPE-UA
ethers	CH_x–O–$\mathrm{CH}_x{}^{a}$	OPLS-UA, OPLS-AA, TraPPE-UA, TAMie
ketones	CH_x–C(=O)–$\mathrm{CH}_x{}^{a}$	OPLS-AA, TraPPE-UA, TAMie
nitriles	CH_x–C≡N^{a}	OPLS-UA, TraPPE-UA
sulfides	CH_x–S–$\mathrm{CH}_x{}^{a}$	OPLS-UA, OPLS-AA, TraPPE-UA
thiols	CH_x–S–H^{a}	OPLS-UA, OPLS-AA, TraPPE-UA

^{a} $x \in [0,1,2,3]$, ^{b} $x \in [0,1,2]$, ^{c} $x \in [0,1]$, ^{d} $X \in$ [H, CH_x].

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